Verification, Validation, and Predictive Capability in Computational Engineering and Physics

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Outline of the Presentation

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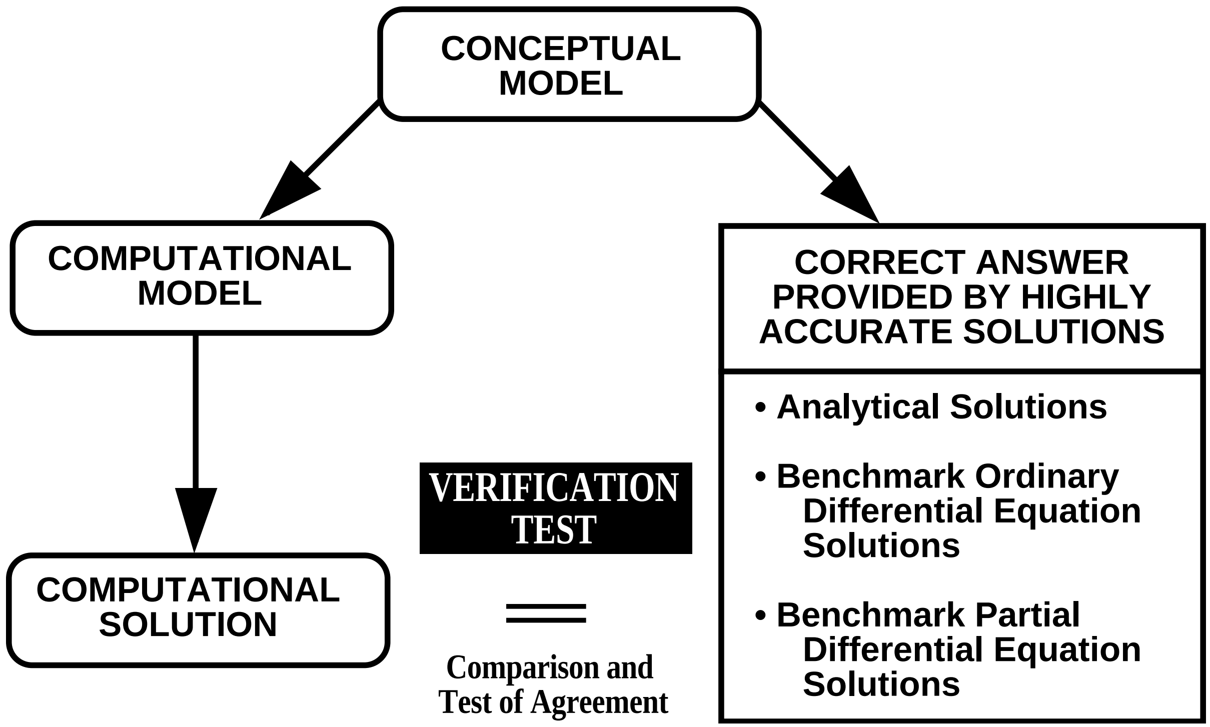
- Introduction and basic terminology
- Relationships between validation and predictive capability
- Development of verification and validation requirements
- Verification activities
- Validation activities
- Predictive capability
- Major research issues
- Major implementation issues
- Concluding remarks

Introduction

- Computational simulations have become a key contributor to:
  - Design and virtual prototyping of engineered systems
  - Supplement physical testing with virtual testing of engineered systems
  - Acquisition of new military systems
  - Certification of the performance, safety, and reliability of high-consequence systems that cannot be tested
- Why are verification and validation (V&V) important?
  - V&V are the primary means of assessing accuracy in computational simulations.
  - V&V are quantitative confidence assessment tools for computational simulations.

AIAA/DOD Definition of Verification

Verification: **The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.**



DOD Definition of Validation

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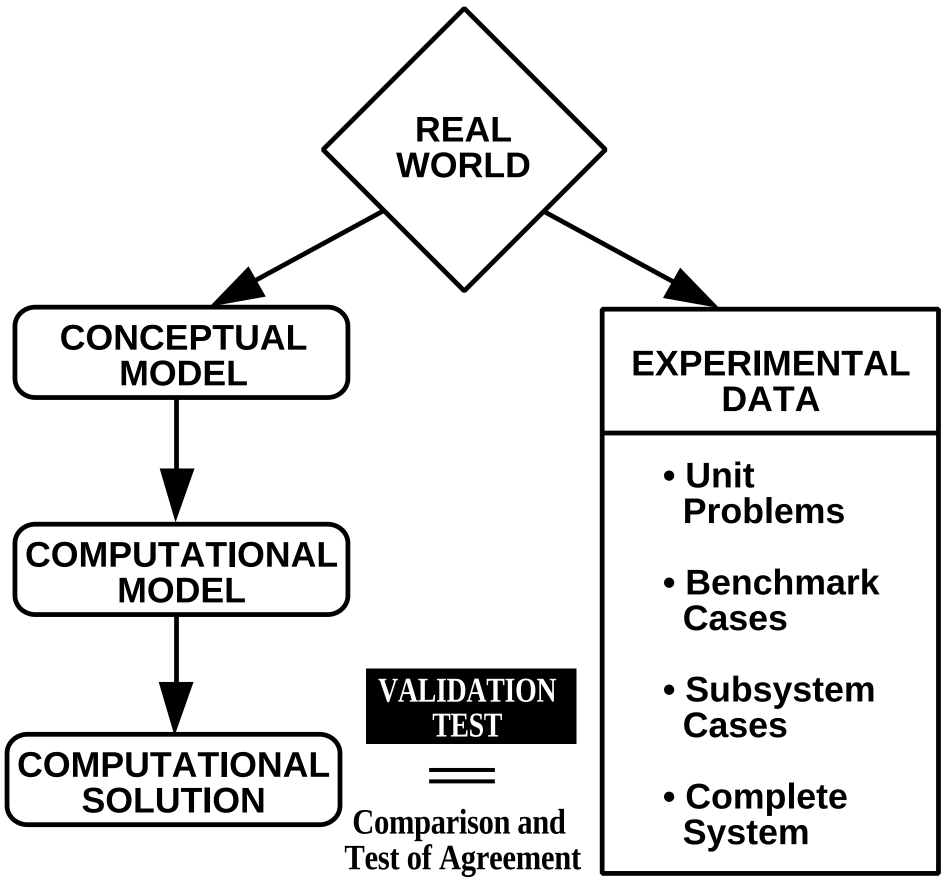
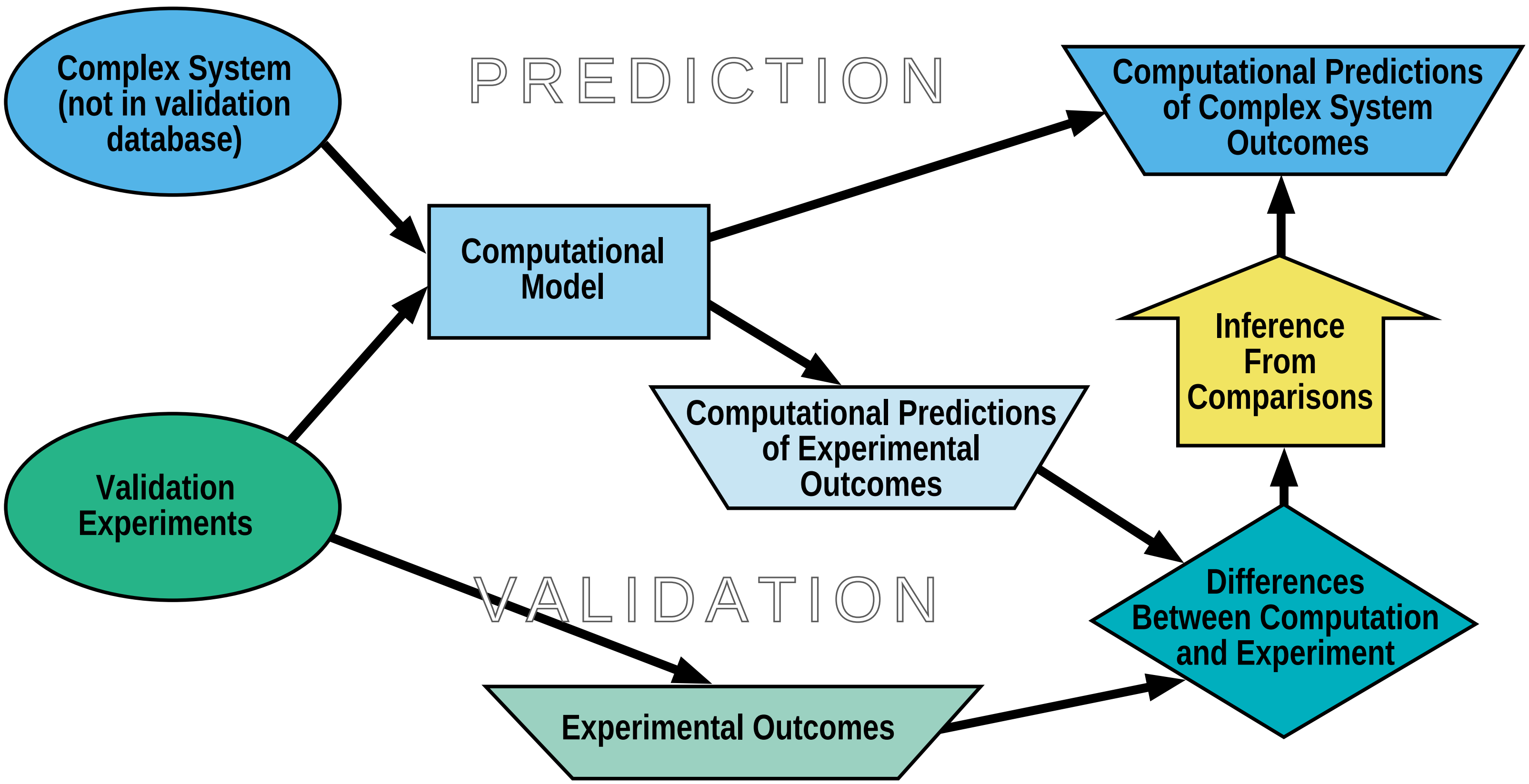
Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.



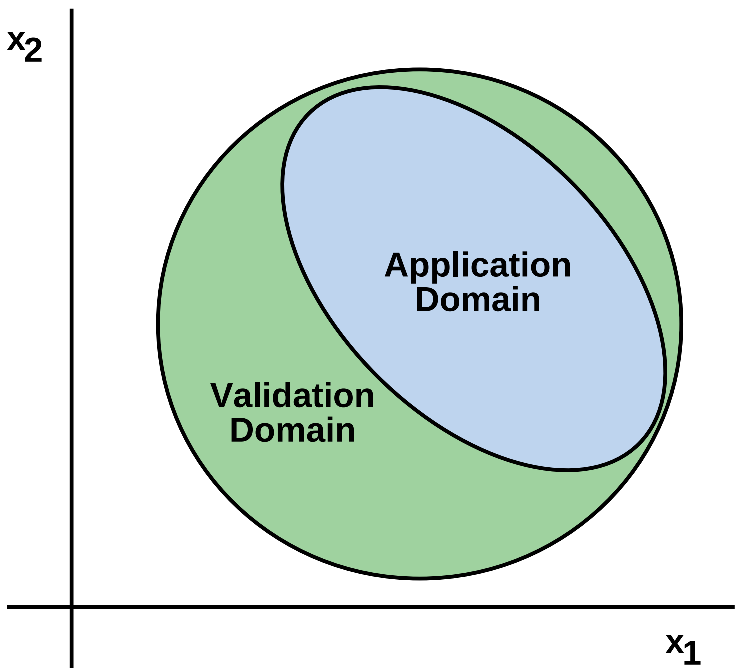
Relationships Between Validation and Predictive Capability

- **Model updating based on previous experimental data (sometimes referred to as “model validation”):**
  - **Properly referred to as parameter identification and model calibration.**
  - **Can use techniques such as Bayesian updating and Markov Chain Monte Carlo methods to determine model parameters.**
  - **Effective for engineered systems “close” to validation experiments.**
- **Alternative approach:**
  - **Appropriate for engineered systems that must operate far from the conditions under which they were validated (or calibrated).**
  - **Requires increased independence between validation and prediction.**
  - **Requires improved quantification of comparisons of computations and experiments: validation metrics**

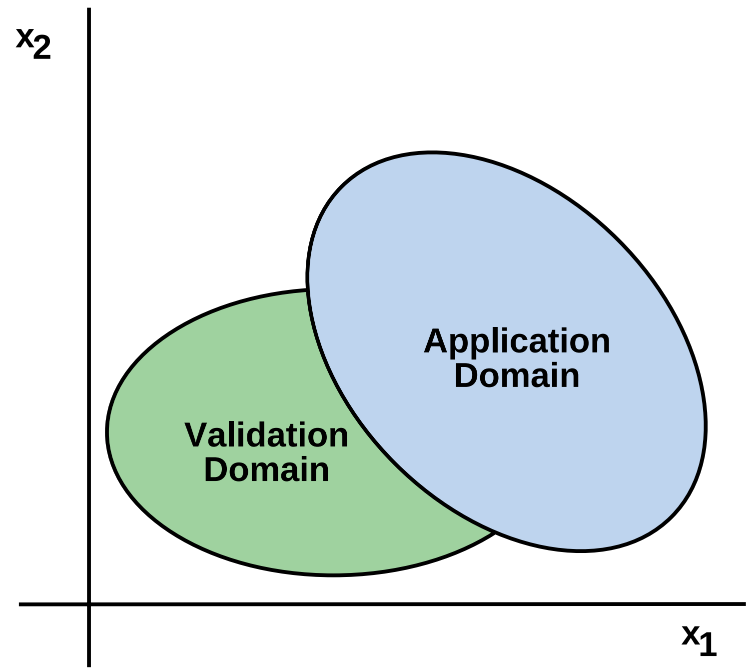
Alternative Relationship of Validation to Prediction



Common Relationships Between Validation Domain and Application Domain



a) Complete Overlap



b) Partial Overlap

Possible Relationship Between Validation Domain and Application Domain

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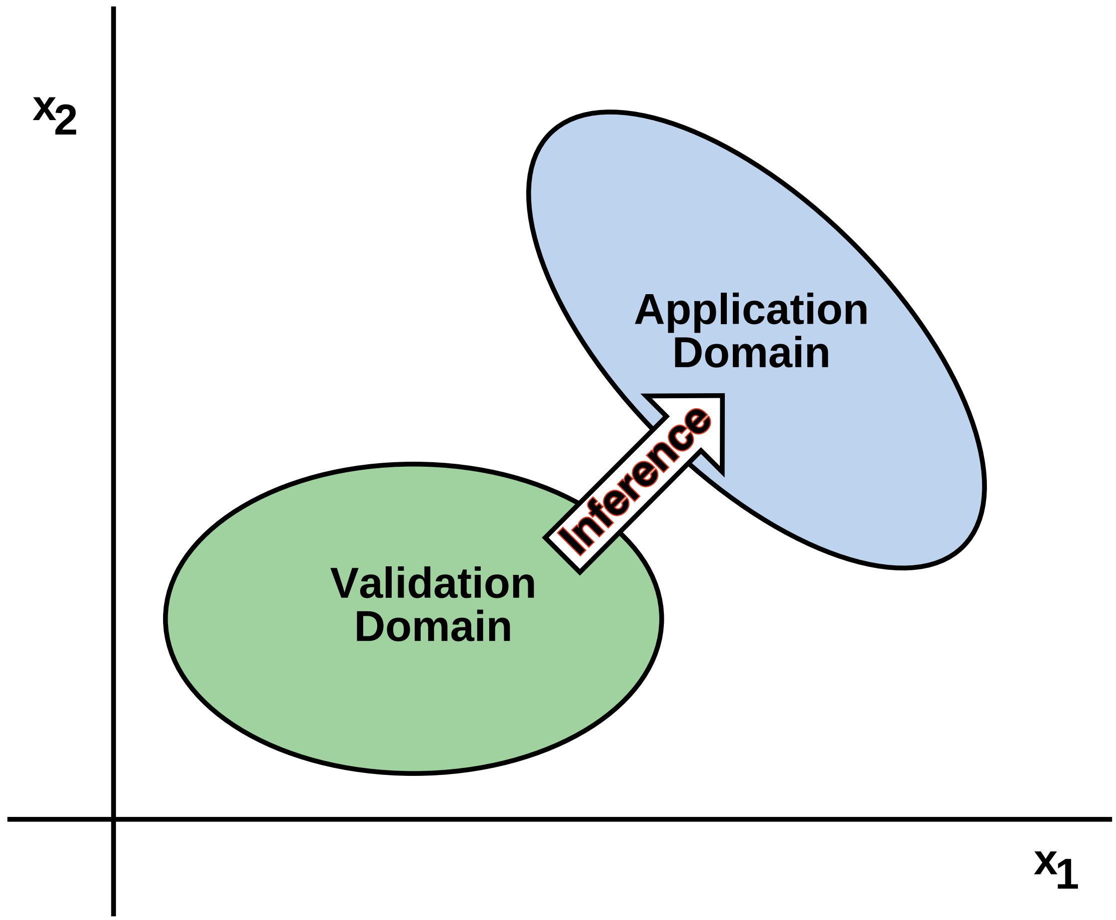

c) No Overlap

Connecting Application Requirements to V&V Requirements

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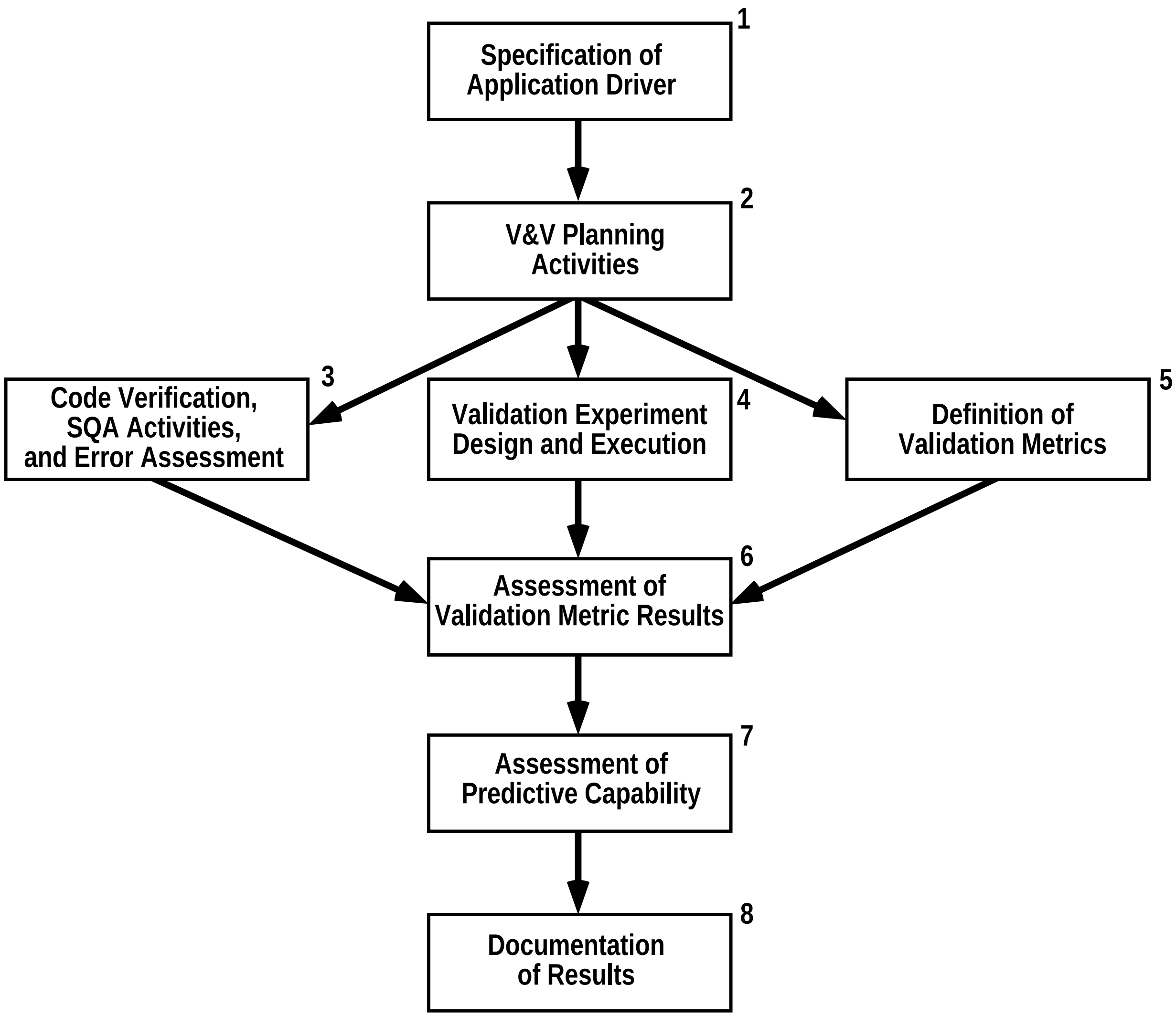
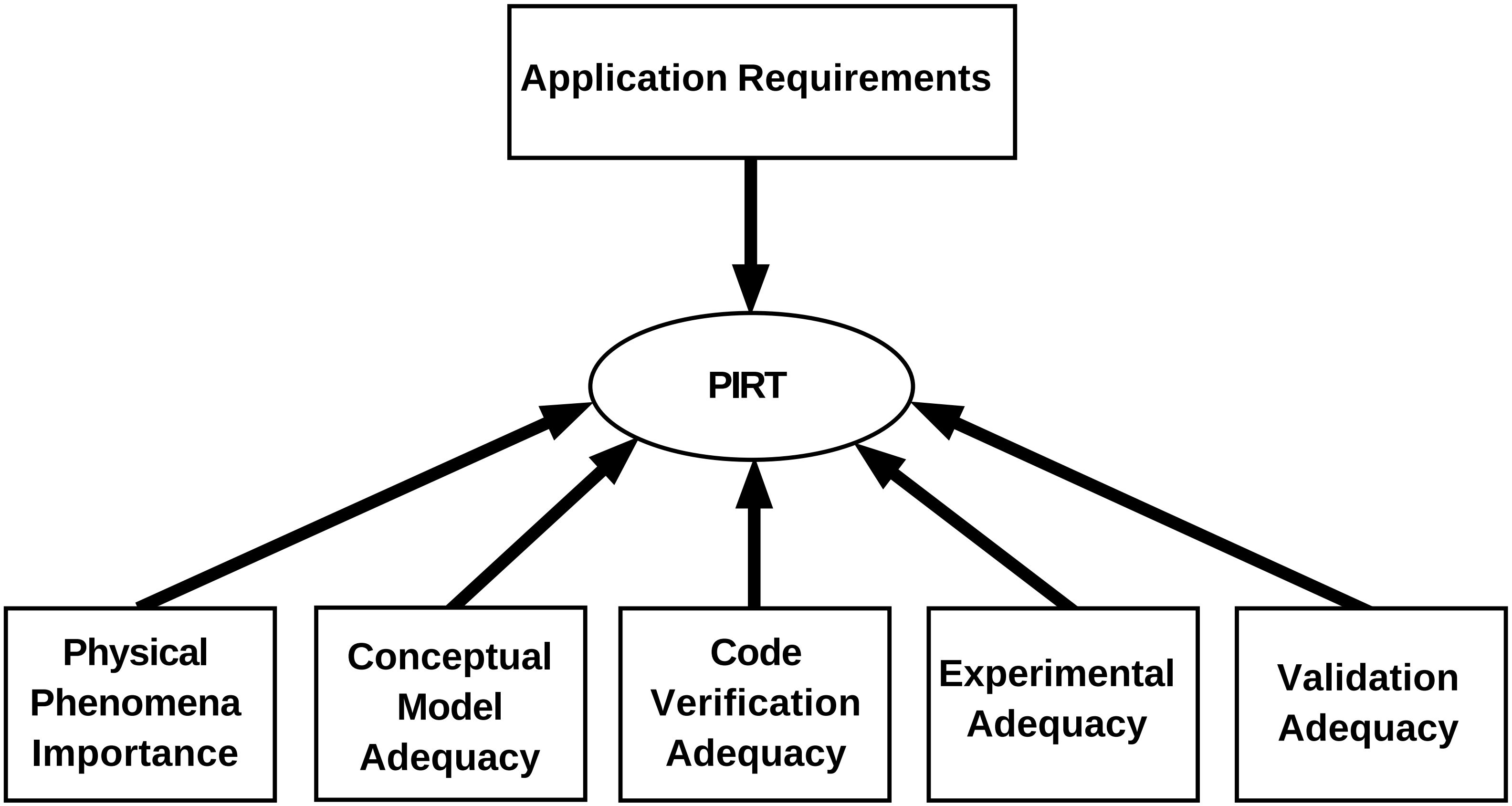


Using PIRT to Determine V&V Requirements and Priorities



Catagories of PIRT Information

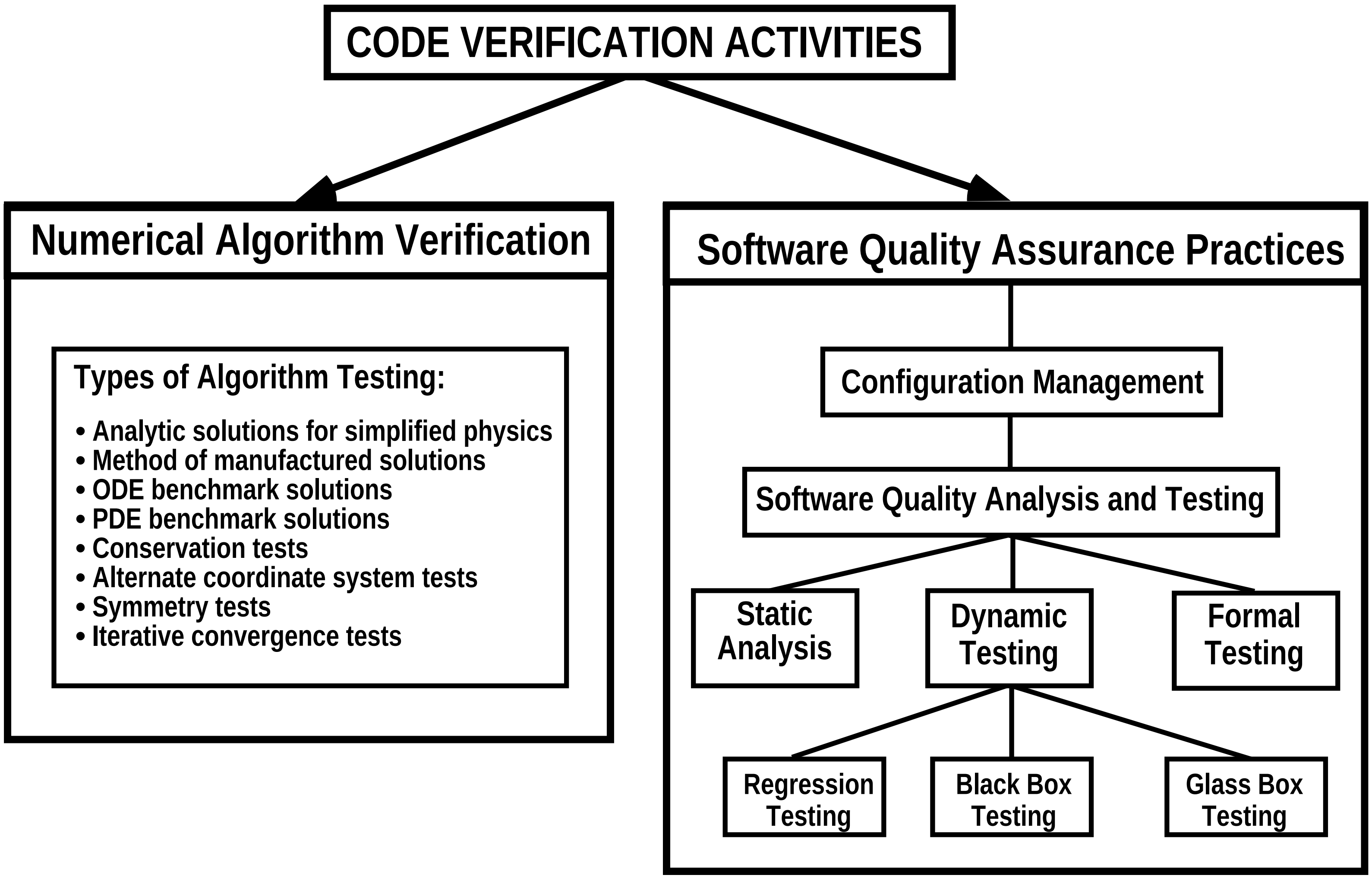
Status of Verification in Computational Physics

- **Hatton studied over 100 scientific production codes over several years. His conclusion:**

  "Scientific calculations should be treated with the same measure of disbelief researchers have for unconfirmed physical experiments."

- **We recommend that verification activities should be divided into three areas:**
  - **Numerical algorithm verification (code verification)**
  - **Software quality assurance (SQA, SQE)**
  - **Numerical error estimation (solution verification)**
- **The goals and tools of each are significantly different.**
- **However, all verification activities should deal only with the observed, i.e., *a posteriori*, performance of the code.**

Integrated View of Verification Assessment



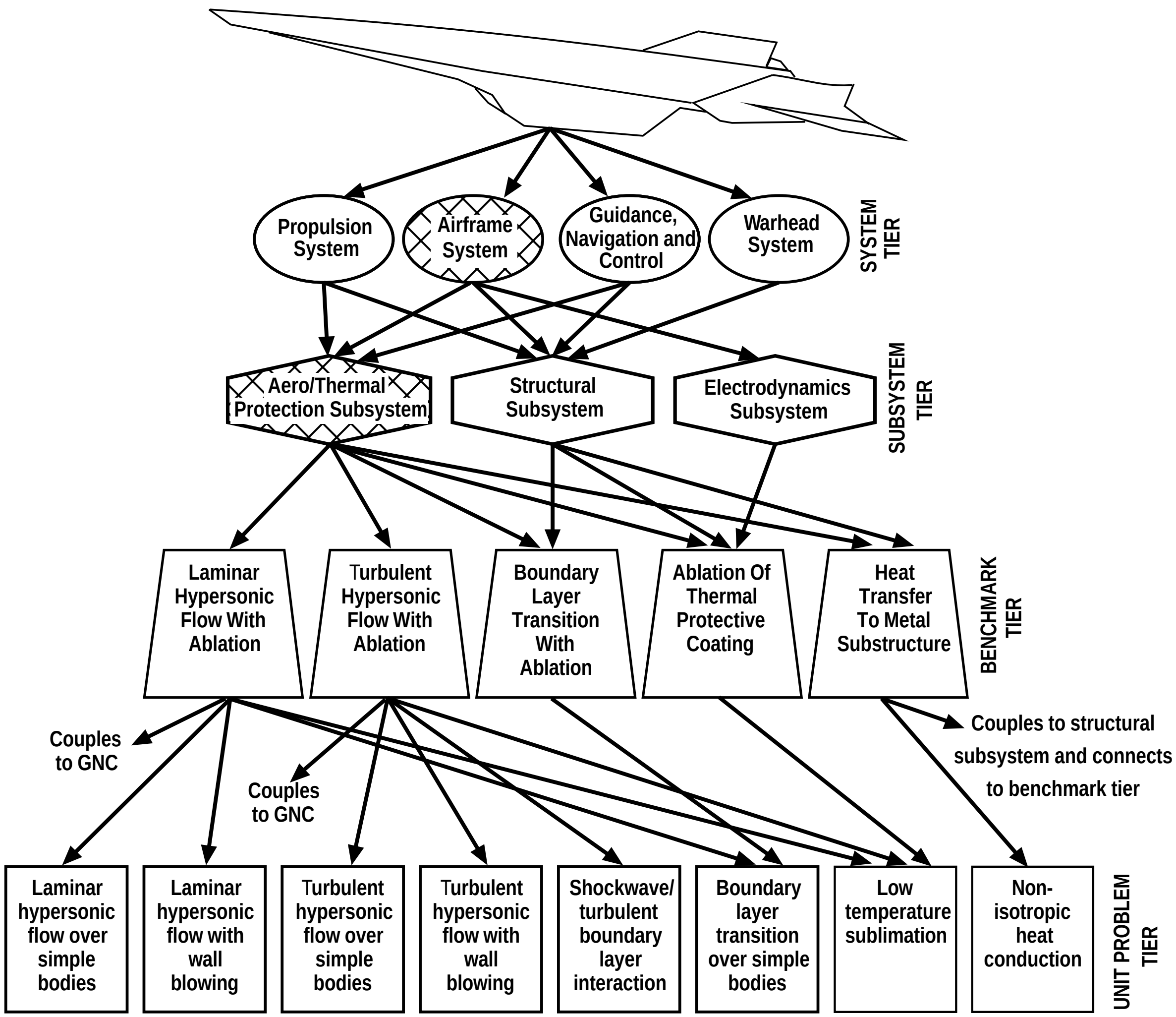
Numerical Error Estimation

- **Insufficient grid and time-step convergence is typically the largest contributor to computational error.**
- ***A posteriori*** **(vs.** ***a priori*****) methods are the only useful methods for estimating error on nonlinear partial differential equations (PDEs).**
- **Two types of grid and time-step error estimation methods:**
  - **Comparison of numerical solutions of the discretized equations on different grid sizes (related to h-adaptivity)**
  - **Comparison of numerical solutions from different discretization methods on the same grid (related to p-adaptivity)**
- **Advantages and disadvantages of each approach:**
  - **Multiple grid solutions are the most accurate and reliable**
  - **Multiple order methods require much less computational effort**

Validation Experiment Methodology: Construction of a Validation Hierarchy

- **Validation hierarchy construction should:**
  - **Carefully disassemble the complete system**
  - **Identify experiments that are attainable and practical**
  - **Identify experiments where validation quality characterization and measurement data can be obtained**
  - **The top of the hierarchy focuses on the application of interest**
  - **The bottom of the hierarchy focuses on separate-effects physics**
- **Phenomena Identification Ranking Table (PIRT) can be used to prioritize individual validation experiments within the hierarchy.**
- **Example:**
  - **Air-launched, air breathing, hypersonic cruise missile**

Hypersonic Cruise Missile



Validation Pyramid for Hypersonic Cruise Missile

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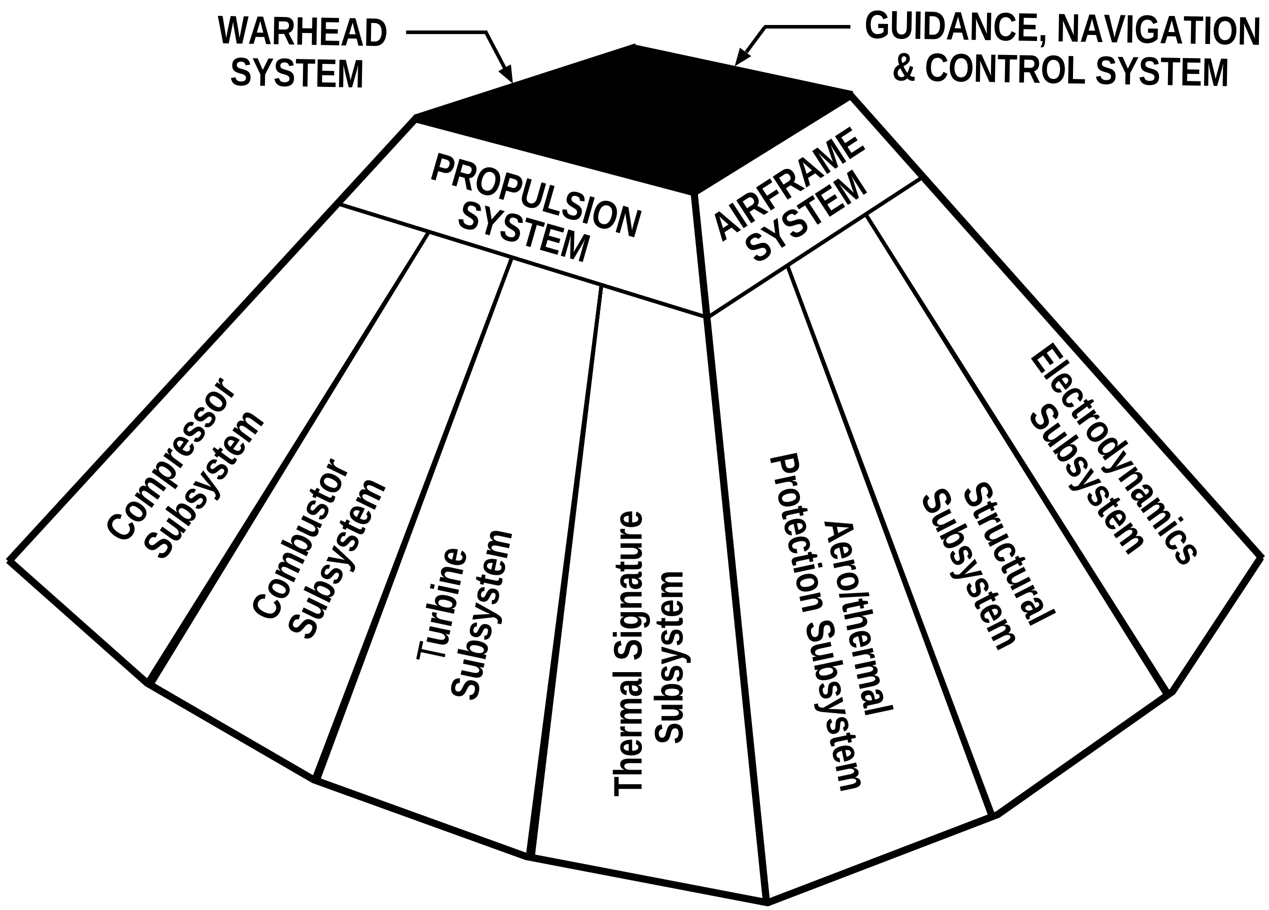

Characteristics of a Validation Experiment

1. **A validation experiment should be jointly designed and executed by experimentalists and computationalists.**

2. **A validation experiment should be designed to capture the relevant physics, all initial and boundary conditions, and auxiliary data.**

3. **A validation experiment should use and develop all possible synergisms between experimental and computational approaches.**

4. **Independence between computational and experimental results should be maintained where possible.**

5. **A hierarchy of experimental measurements should be made that presents an increasing range of computational difficulty.**

6. **Develop and employ experimental uncertainty analysis procedures to delineate and quantify random and bias errors.**

Validation Quantification

- **Approaches to validation quantification:**
  - **Model updating**
  - **Hypothesis testing**
  - **Comparison of computation and experiment**
- **Each approach relies on statistical measures because of:**
  - **Random experimental measurement error**
  - **Uncontrolled experimental parameters needed as input for computational simulations**
  - **Unmeasured experimental parameters needed as input for computational simulations**
- **We refer to the comparison of computation and experiment as a validation metric.**

Increasing Quality of Validation Metrics

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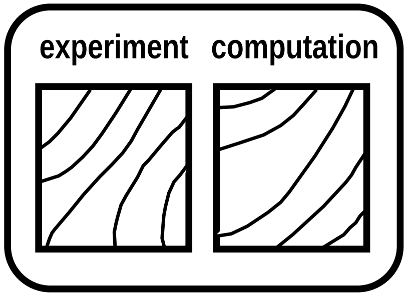
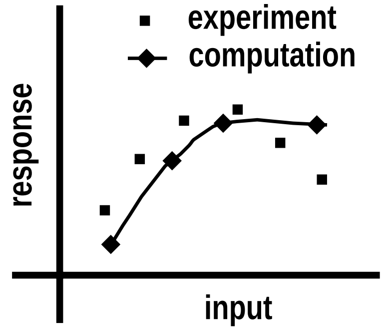
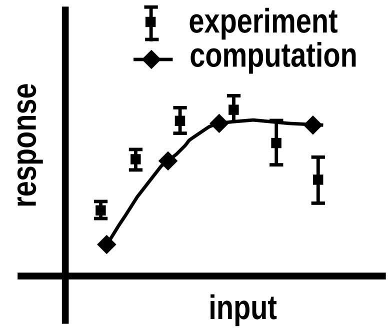


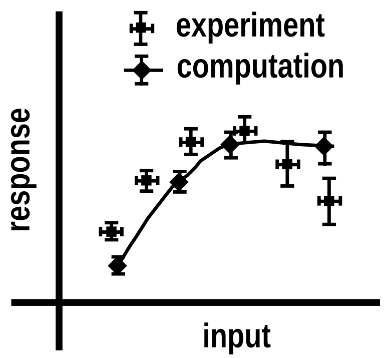
(a) Viewgraph Norm



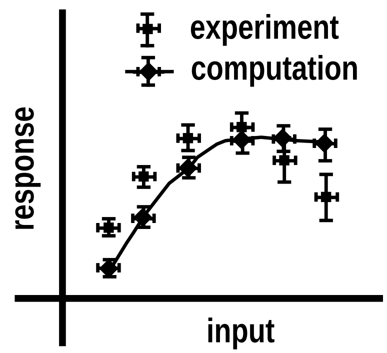
(b) Deterministic



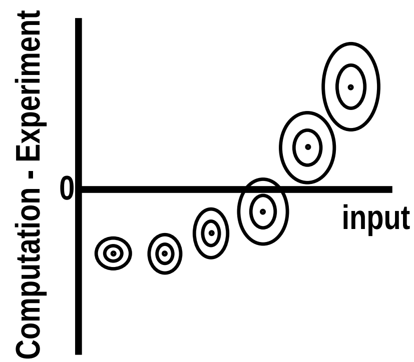
(c) Experimental Uncertainty



(d) Numerical Error



(e) Nondeterministic Computation



(f) Quantitative Comparison

Recommended Features for Validation Metrics

- **Features that should be included in a validation metric:**
  - **Should include an estimate of the numerical error.**
  - **Should include an estimate of the experimental random errors and the correlated bias errors.**
  - **Should include a test of the modeling assumptions.**
  - **Should only provide a measure of agreement between computation and experiment (not a measure of adequacy for future applications).**
  - **Should depend on the number of experimental replications of a given experimental quantity.**
  - **Should include uncertainty due to lack of experimental measurement of needed computational quantities and random uncertainty in experimental parameters.**

Predictive Capability: Uncertainty and Error

- **Uncertainty and error are commonly used interchangeably in computational physics.**
- **A number of researchers have argued that uncertainty and error should be clearly separated.**

Error: A recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge.

- **Acknowledged errors can be estimated, bounded, or ordered.**
  (discretization error, iterative error, geometry approximations)
- **Unacknowledged errors are mistakes or blunders.**
  (source code errors, compiler errors, incorrect input or output files)

Predictive Capability: Uncertainty

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Uncertainty: **A potential deficiency in any phase or activity of modeling process that is due to lack of knowledge.**

- **Risk assessment and information theory communities segregate uncertainty into:**
  - **Aleatory uncertainty (variability, randomness, irreducible uncertainty)**
  - **Ex: Random variation in thermodynamic properties, joint stiffness and damping due to manufacturing variability**
  - **Epistemic uncertainty (lack of knowledge uncertainty, model form uncertainty, reducible uncertainty)**
  - **Ex: poor understanding of turbulent-reacting flow and fracture dynamics, and lack of knowledge of deeply buried target characteristics**

Uncertainty and Error in Computational Predictions

- **Sources of uncertainty in computational predictions:**
  - **Validation metric will (hopefully) be a statistical measure**
  - **Conditions for the prediction will typically involve both aleatory and epistemic uncertainty**
  - **Alternate plausible models of the physical process**
- **Quantities needed for input to the predictions:**
  - **Input parameters (e.g., material properties, transport properties)**
  - **Initial conditions (e.g., initial fluid temperature, bolt preloads)**
  - **Boundary conditions (e.g., inflow conditions, forcing function)**
- **These uncertainties are normally mixed with numerical errors.**
- **Nondeterministic simulations are required to construct an ensemble of computations for a prediction.**

Three Steps for Nondeterministic Simulations

1) For the unknown or experimentally uncontrolled value construct a probability distribution.

   - Probability distributions are either determined experimentally, or assumed.

Characterizing the source of the uncertainty

2) Select input values using statistical sampling procedures.

   - Monte Carlo or Latin Hypercube procedures are typically used.

Uncertainty propagation through the computational model

3) From multiple individual computations, construct probability distributions of the required output quantities.

   - Multiple computational realizations are statistically compared with the experimentally measured quantities.

Uncertainty quantification in the computational result

Major Research Issues: Prioritization of Assessment Activities

- **The Phenomena Identification and Ranking Table (PIRT) has proven to be the most effective method for prioritization of V&V activities.**
- **PIRT can incorporate relative importance and adequacy:**
  - **Importance of multiple phenomena**
  - **Importance of multiple applications**
  - **Adequacy of alternative conceptual models**
  - **Adequacy of verification activities**
  - **Adequacy of validation simulations**
  - **Adequacy of validation experiments**
- **Methods for combining relative importance and adequacy need to be developed and evaluated.**

Major Research Issues: Prioritization of Assessment Activities

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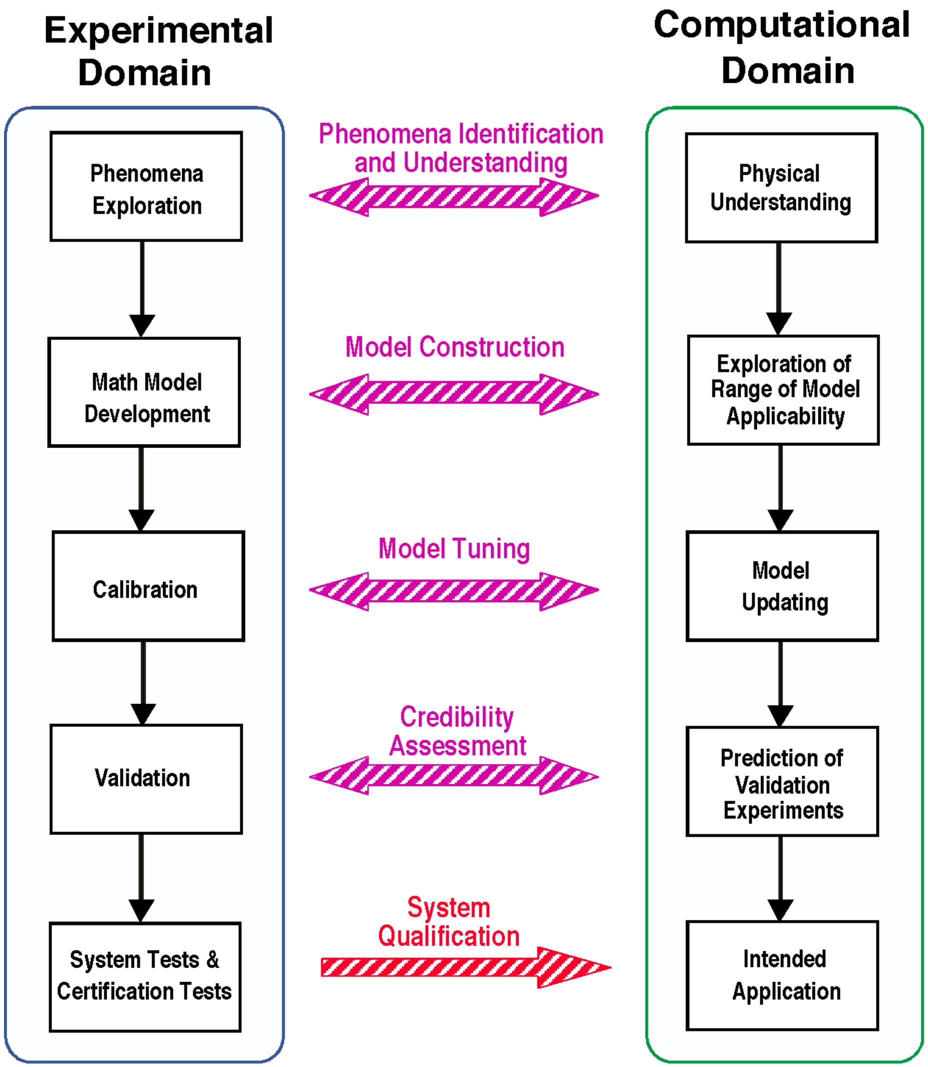

Major Research Issues: Verification Activities

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- **The Method of Manufactured Solutions (MMS) should be developed more broadly:**
  - **Within the disciplines where it is already used, e.g., shock waves, multiphase flow, free-surface flows, and large-eddy simulation**
  - **Across more disciplines, e.g., large plastic deformation, fracture dynamics, radiation transport, and electromagnetics**
  - **Proper treatment of boundary conditions for mixed elliptic, parabolic, and hyperbolic PDEs**
- **Development of verification methods for non-unique solutions of nonlinear PDEs:**
  - **Solution bifurcation of elliptic PDEs**
  - **Chaotic solutions of hyperbolic PDEs**

Major Research Issues: Validation Activities

- **Further development and use is needed of the validation hierarchy and the system validation pyramid.**
- **Development of methods is needed to assess the adequacy, relative to the intended application, of:**
  - **Formulation of the validation metric itself**
  - **Numerical value of the metric**
- **Both tasks will be difficult because application requirements for metrics are:**
  - **Commonly not known or firm at the higher levels of the validation hierarchy**
  - **Rarely known for lower levels in the validation hierarchy**

Major Research Issues: Validation Activities (continued)

- **Additional research is needed in the formulation of validation metrics:**
  - **For steady-state problems, metrics constructed over 2D and 3D fields**
  - **For unsteady problems, formulate metrics in time**
  - **For unsteady problems with eigen frequencies, formulation of metric in the frequency domain**
  - **Methods for propagating metrics at lower levels of the validation hierarchy to higher levels of the hierarchy**
- **Bayesian updating and other calibration methods should provide additional ideas for formulation of metrics.**
- **Research is needed into determining measures of “distance” between a validation experiment and an application condition.**

Major Implementation Issues: Management Issues

- An adversarial or competitive relationship may exist between computationalists and experimentalists, either within or between organizations.
- Management must:
  - Become aware of adversarial or competitive relationships
  - Avoid any inadvertent endorsement of adversarial or competitive relationships
  - Promote synergistic relationships
- Improved methods should be found for presenting concise quantitative measures of V&V maturity.
- Verification and validation dial-meters for codes and calculations show significant promise to show relative status.

Major Implementation Issues: Management Issues (continued)

- **Management must recognize the importance of nondeterministic simulations for validation metrics and in predictive capability**
- **Systems that have heavily relied on computational simulation for safety certification requirements have fully accepted this approach:**
  - **Nuclear reactor safety**
  - **Underground storage of nuclear wastes**
- **Management must find ways to emphasize or quantify the value added by V&V activities.**
- **Factors that could be used to emphasize/quantify value added by V&V:**
  - **Professional risk to the code user of software inaccuracy/failure**
  - **Organizational risk of software inaccuracy/failure, e.g., company liability cost, environmental damage, and national security impact**

Major Implementation Issues: Industrial Setting

- **Difficulties of commercial code validation in an industrial setting:**
  - **Range of accuracy requirements between customers is very large**
  - **Split responsibility for validation between industrial users and commercial code company**
- **Industrial users must commonly deal with a complex mixture of errors and uncertainties:**
  - **Under-resolved grids**
  - **Poor grid quality**
  - **Inadequate iterative convergence**
  - **Calibration of physical model parameters**
- **Industrial users attempt to manage uncertainties and rely on the computation of incremental changes from their databases: use of deltas**

Major Implementation Issues: Commercial Software

- **Difficulties of implementing V&V procedures for commercial codes:**
  - **Code verification and SQA activities for a very wide range of computer hardware, system software, and complier software.**
  - **V&V cannot be completely tested for all possible combinations of input and output options, and internal options available in commercial software.**
  - **Bug finding, fixing, tracking, and reporting is much more difficult**
- **Documentation and availability of V&V activities of commercial software has been, in general, very poor.**
- **Electronic documentation, either in the commercial software or on the web site of the commercial software company, is recommended.**
- **User training and support of commercial software companies should be the model for industrial developed software.**

Major Implementation Issues: Development of Standards

- **Attempts should be made to standardize the meaning of validation:**
  - **Validation does not imply adequacy for applications: fidelity assessment**
  - **Validation implies adequacy for specified applications: DOD view-point**
- **Need for industry-wide standards for V&V terminology, procedures, and tools:**
  - **Professional engineering societies**
  - **Important role of European Research Community on Flow, Turbu-lence, and Combustion (ERCOFTAC) and National Agency for Finite Element Methods and Standards (NAFEMS)**
  - **These efforts should be discipline specific and should be com-posed of a very broad constituency.**

Major Implementation Issues: Development of Standards (continued)

- **Compilation, generation and documentation of highly accurate solutions for code verification should be initiated:**
  - **Sometimes referred to as strong-sense benchmarks**
  - **Role for professional engineering societies, academic institutions, nonprofit organizations, and commercial software companies.**
- **Compilation, generation and documentation of validation databases should be initiated:**
  - **Attempts have been made by the AIAA CFD Committee on Standards and National Project for Applications-oriented Research (NPARC) in CFD**
  - **Thematic Network on Quality and Trust for the Industrial Applications of CFD (QNET-CFD) is has 40 participants from several countries**
  - **QNET is funded by the European Commission**

Closing Remarks

- **Code verification on scientific and engineering software is in a dismal state, based on the comprehensive study of Hatton.**
- **Prioritization of V&V activities must be done.**
- **Validation experiments are significantly different than traditional experiments: The code is the customer**
- **Much of the existing validation experimental data will prove to be inadequate for quantitative validation**
- **New validation experiments will be costly and they will present risks to experimental facilities**
- **Validation experiments must have close cooperation between experimentalists and computationalists.**
- **The primary goal in validation is assessing the accuracy of models: not fixing or improving models.**

Closing Remarks (continued)

- **Users of the codes and users of the results of codes should require detailed documentation of V&V activities.**
- **We must find ways of convincing commercial software companies to share information on the V&V procedures they use.**
- **Industrial settings commonly require mixtures of large numerical errors and large modeling uncertainties: calibration of models must be done with extreme care.**
- **V&V activities are commonly supported as long as they:**
  - **Don't cost the code development project too much money**
  - **Don't negatively impact the code development schedule**
- **V&V activities provide short term and long term value added.**
- **We do not believe a "V&V inspection approach" will be effective.**